1-Butanol, 3-methoxy-3-methyl-, acetate 103429-90-9 | DTXSID30145852

103429-90-9	DTXSID30145852

Model Performance

_			
N	Model	Data	

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 2.15

Global applicability domain: Inside

Local applicability domain index: 5.81e-01

Confidence level: 7.59e-01

Nearest Neighbors from the Training Set

Image not found

2-Isopropyl-6-methyl-4-

pyrimidone Measured: 1.82 Predicted: 2.23 Image not found

Paraldehyde Measured: 3.02

Predicted: 2.77

Image not found

Bromacil

Measured: 3.24 **Predicted:** 2.87

Image not found

4-Isobutylmorpholine

Measured: 1.78 Predicted: 2.69

Image not found

Dimethoate
Measured: 1.58
Predicted: 1.88